BASIC MODELING OF THE SOLAR ATMOSPHERE AND SPECTRUM

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Final Report

For the period 1 July 1997 through 30 June 2000

Principal Investigator

Dr. Eugene H. Avrett

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> Smithsonian Institution Astrophysical Observatory Cambridge, Massachusetts 02138

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1. Introduction

During the last three years we have continued the development of extensive computer programs for constructing realistic models of the solar atmosphere and for calculating detailed spectra to use in the interpretation of solar observations. This research involves two major interrelated efforts: work by Avrett and Loeser on the Pandora computer program for optically thick non-LTE modeling of the solar atmosphere including a wide range of physical processes, and work by Kurucz on the detailed high-resolution synthesis of the solar spectrum using data for over 58 million atomic and molecular lines. Our objective is to construct atmospheric models from which the calculated spectra agree as well as possible with high- and low-resolution observations over a wide wavelength range. Such modeling leads to an improved understanding of the physical processes responsible for the structure and behavior of the atmosphere.

We deal with different brightness regions on the solar disk by calculating models

for 7 separate spatial components:

A Faint regions of network-cell interiors

C Average network-cell regions (average quiet Sun)

E Average network lanes

F Bright network lanes

H Average plage areas

P Bright plage areas

S Large sunspot umbrae

To a first approximation, such different types of features can be treated separately, assuming little interaction between the different features, since their horizontal extent is usually much larger than the vertical distance between the photospheric and coronal layers in each case. Hence, it is reasonable as a first approximation to construct separate one-dimensional models that describe the vertical structure of each horizontally distinct region.

The modeling provides a way of calculating spectral irradiances at wavelengths throughout the spectrum based on images of the disk that show the distribution of

quiet and active regions at any time.

To the extent that our calculated spectra for various brightness components of quiet and active regions agree with corresponding observations at high spatial (but low temporal) resolution, our simulations can be used to relate the intensity at one wavelength to that at any other wavelength in quiet or active regions anywhere on the disk. Using available disk images in the Ca K, Ha, and He 1083 nm lines to establish the detailed distribution of quiet and active regions on the disk at a given time, we can calculate the corresponding images at any wavelength in the UV or EUV, and then integrate to obtain any needed UV or EUV spectral irradiances.

Changes in the ozone concentration and other chemical properties of the Earth's upper atmosphere are observed to be correlated with UV and EUV solar irradiance variations on time scales from a few days up to the 27-day period of solar rotation. Direct UV and EUV irradiance measurements during the last two 11-year solar activity cycles have been too few in number and too uncertain in absolute calibration to determine how much the solar input affects the molecular chemistry high in the Earth's atmosphere. Our theoretical spectra now seem accurate enough so that we can use the available ground-based images to determine the past record of UV and EUV spectral

irradiances.

We are collaborating with O. R. White, J. M. Fontenla, and P. A. Fox in Boulder on the calculation of solar irradiances and the comparison between our simulations and observed irradiances. Our role in this project is to produce a set of atmospheric models for the observed range of quiet and active regions, and to calculate for each model the intensity spectrum at all wavelengths of interest as a function of heliocentric position on the solar disk. The Boulder group is using these results to construct UV images, and the corresponding irradiances, based on visible disk images and magnetograms which show the distribution of quiet and active regions at any given time. They are comparing the calculated spectral irradiances in the 120-420 nm wavelength range to the irradiances at various times observed with the UARS SOLSTICE satellite instrument. Our first paper reporting on these results has been published in the Astrophysical Journal by Fontenla, White, Fox, Avrett, and Kurucz (1999). See also Avrett (1998).

As far as possible, our modeling is based on simulating the detailed physical processes that are thought to be important in the solar atmosphere, not on merely adjusting model parameters to fit observations. The methods and assumptions used in our calculations are discussed in Section 3 below. Discrepancies between calculated and observed intensities lead us to identify new processes that must be taken into account.

2. Models

Hydrogen is almost completely neutral in the photosphere and low chromosphere, but starts to become ionized as the temperature increases and the density decreases. As the temperature reaches about 8000 K, radiative cooling by the strong Lyman α line becomes important, and initially acts to limit higher temperatures. The temperature must then increase abruptly to cause hydrogen to be almost fully ionized, since if the temperature increased gradually, the Lyman α line would radiate away more energy than could be provided by any plausible source of local non-radiative heating. Only about 1 part in 10⁴ of the radiative energy emerging from the photosphere is needed as non-radiative heating to cause the temperature to rise in the chromosphere (see Athay 1988). Only about 1 part in 105 of the total energy from the photosphere is needed to form the transition region and corona. Of this, a small fraction escapes as coronal line radiation and most of the rest is transported down to lower temperatures by thermal conduction, particle diffusion, and mass flows, to provide the energy emitted in the hydrogen and helium resonance lines. See Fontenla, Avrett, and Loeser (1993) and Avrett (1999). Only about 10 km separates the top of the chromosphere where T=104K and the lower corona where T=105K. We describe the transition region in terms of a one-dimensional stratification even though it appears to be an undulating sheet that occurs at various heights and orientations above the photosphere.

Coronal line radiation at wavelengths shortward of the He I ionization edge at 50.4 nm illuminates the upper chromospheric layers and causes weak ionization of He I followed by recombination, thus strengthening the absorption of the photospheric continuum by the He I lines at 587 and 1083 nm on the disk. Images of quiet reagions of the Sun just above the limb show a narrow band of helium line emission at an almost uniform height of about 2000 km above the photosphere, but this He I emission weakens or disappears in coronal hole regions, i.e., where the coronal illumination weakens (see Avrett, Fontenla, and Loeser 1994 and references therein). Thus, over much of the quiet Sun seen at the limb, the top of the chromosphere seems to occur where the density drops abruptly at a height of roughly 2000 km, but often there are much higher projections of neutral material in loops, and spicules, and prominences (see Fig. 2 of Fontenla, Avrett, and Loeser 1993).

Average models cannot account for the spatial features on the Sun that are brighter or fainter than average regions. We have constructed separate models for the different brightness components that are observed with high spatial resolution. Models A, C, and F indicate that the 110 nm continuum of C I for all three quiet-Sun brightness components is formed in the middle of the chromosphere at a height of about 1200 km. The temperature difference between models A and F at this height is only about 170 K, even though the intensities differ by almost a factor of 4. Without contrary evidence, one might conclude that models A and F represent approximate lower and upper bounds on the time-averaged temperature distribution for the various components of the quiet Sun, if indeed the models are based on valid assumptions.

The infrared CO lines appear to offer such contrary evidence, at least for heights up to about 1000 km. The strongest of these lines have central brightness temperatures of 4100 K at disk center and lower values near the limb. These lines are formed in LTE, according to Ayres and Wiedemann (1989), so that the observed brightness temperature is roughly the temperature at the depth of formation. As discussed by Avrett (1995), a hydrostatic-equilibrium model based on the CO lines alone has a temperature of 4100 K at a height of about 700 km, and lower temperatures at greater heights. The CO lines do not show any evidence of the chromospheric temperature rise that is indicated by other line and continuum diagnostics. These infrared CO observations appear to be inconsistent with observations of UV chromospheric lines at high spatial and temporal resolution by Carlsson, Judge, and Wilhelm (1997) which show that while the UV line emission varies with time and position, it never vanishes. implying that the chromospheric temperature rise is persistent and not the time average of transitory increases in temperature, as proposed by Carlsson and Stein (1995). Waves traveling through the atmosphere produce temperature variations with time, and CO line absorption is greatly enhanced at low temperatures and diminished at high temperatures. Evidence for such time variations is provided by the observations of Uitenbroek, Noyes, and Rabin (1994) and Uitenbroek and Noyes (1994) who obtained spatially and temporally resolved CO spectra near 4.67 μm with a new infrared array detector at the McMath-Pierce solar telescope at Kitt Peak. See also Avres (1995, 1998) and references therein. Fig. 2 of Uitenbroek and Noves (see also Uitenbroek 1999) shows a space-time map of the 3-2 R14 linecore brightness temperature along a 94 arcsec slit placed over a quiet region near disk center during a period of 23 minutes. They found peak-to-peak temperature fluctuations of approximately 400 K, and substantial time variations at each position. Dark areas usually become much brighter within 1 to 3 minutes. These observations clearly show that dynamical effects play an important role in determining the low brightness temperatures seen in the cores of the strong infrared CO lines.

As reported by Avrett, Höflich, Uitenbroek, and Ulmschneider (1996), we have studied the effects of acoustic waves traveling through the chromosphere, solving the hydrodynamic equations with the method of characteristics, and including non-LTE radiative transfer and the time-dependent rate equations for the formation of CO. We find that while the fine-structure levels of the rotation-vibration bands are populated according to LTE (Ayres and Wiedemann 1989), the total amount of CO cannot follow rapid temperature changes. Typical time scales for the formation of CO range from a minute at a height of 100 km to hours at 1000 km, i.e., much longer than typical hydrodynamic time scales. Thus the total CO concentration effectively corresponds to a time-averaged temperature structure, while the relative populations of the fine structure levels are in LTE corresponding to the instantaneous local temperature.

Uitenbroek (1999) has carried out an analysis of the infrared CO lines observed at high spatial and temporal resolution using multi-dimensional radiative transfer modeling to study the formation of these lines at one given time from a hydrodynamic granulation simulation by Stein and Nordlund (1989). These calculations suggest that if the CO concentration in the hot convective upflow regions cannot increase fast

enough to follow the decrease in temperature as these regions cool in the higher layers above the photosphere, then these lines would form deeper than in one-dimensional hydrostatic-equilibrium models and would be more in agreement with the observations. Thus, the strong infrared CO lines would be formed in the temperature minimum region and would not be expected to show chromospheric emission.

This explanation would remove one of the difficulties that the shock wave models of Carlsson and Stein (1995) attempted to resolve. Their successful modeling of observed Ca II bright points gave as a byproduct an intermittent chromosphere lacking the persistent outward temperature increase of time-average empirical models that is needed to explain the observations of UV emission lines and continua. Kalkofen, Ulmschneider, and Avrett (1999) find that their model calculation provides only about one percent of the acoustic energy that heats the chromosphere, and identify dissipation by short-period (P < 100s) acoustic waves as the likely mechanism by which the chromosphere is heated, resulting in a persistent outward average temperature increase.

3. Methods

The Pandora computer program (Avrett and Loeser 1992) is a general-purpose non-LTE rediative transfer program for atmospheric modeling and line profile calculation. For a static one-dimensional atmosphere or one with an arbitrary inward or outward stratification of velocity the program is used to solve the various equations describing the optically thick non-LTE transfer of line and continuum radiation for multilevel atoms and multiple stages of ionization, with line interlocking and partial frequency redistribution, subject to the effects of incident illumination, non-radiative heating, radiative energy balance, hydrostatic or pressure equilibuium, and the effects of non-Maxwellian particle diffusion in addition to mass outflow and mass inflow. It relies upon Kurucz's comprehensive set of atomic and molecular line opacities in calculating photoionization and photodissociation rates, and on his detailed spectrum synthesis programs to compute a theoretical solar spectrum.

The Pandora program was used by Vernazza, Avrett, and Loeser (1981) to determine models corresponding to the brightness components of the quiet Sun from Skylab observations in the EUV wavelength range 40-140 nm. The temperature distribution for each component was adjusted empirically to obtain agreement between calculated and observed intensities. Fontenla, Avrett, and Loeser (1993) replaced the empirically determined transition regions in these models by theoretical energy balance models that include the effects of energy transport by particle diffusion. Further development of the Pandora program, reported by Avrett (1999), allows mass outflows and mass inflows to be treated in detail, including for the first time the effects of optically-thick non-LTE radiative transfer in such mass-flow cases, which substantially alters the ionization balance of the various species in the transition region.

While we can determine the chromospheric temperature structure by means of a prescribed mechanical heating function, as did Anderson and Athay (1989), we have continued to adjust the chromospheric temperature distribution empirically to get best agreement with the observations and then to calculate what the corresponding mechanical heating would be. A major uncertainty is how to systematically treat the departures from LTE in the millions of absorption and emission lines throughout the spectrum. Anderson (1989) proposed a general scattering albedo formula based on his detailed study of the Fe I and Fe II lines. We have found that in the temperature minimum region and low chromosphere the lines are much closer to LTE than this formula predicts, presumably due to the large numbers of molecular lines. Our current approach is to use Pandora to calculate the departures from LTE for the principal energy levels of atoms and ions as input to Kurucz's detailed simulations. At present

only H I, H-,He I, He II, Li I, B I, C I, C III, C III, C IV, O I, O II, Na I, Mg I, Mg II, Si II, Si III, Si III, S I, K I, Ca I, Ca II, and Fe I are computed. Approximate source functions are used for other species. We expect to add many more ions during the course of this work.

Kurucz has been making detailed comparisons of our current calculated intensity spectra to FTS observations in the visible and to SUMER (Brekke 1996; Curdt et al.

1999) and earlier spectra in the ultraviolet.

Kurucz is attempting to provide all of the basic atomic and diatomic molecular data needed to compute opacities, model atmospheres, and spectra for the Sun and other stars. For opacity and model atmosphere calculations where only statistical accuracy is needed, the current list of 58 million lines, most with predicted wavelengths, works reasonably well. However, when computing spectra intended to match the solar spectrum, using only the lines with accurate wavelengths, the quality is poor since roughly half of the observed lines are missing. Most of the gf values need to be corrected, and even the laboratory wavelengths are not always reliable. In addition, hyperfine and isotopic splitting must be included because this splitting significantly broadens many lines.

To improve the correspondence between the calculated and observed spectra, Kurucz collects all published data on gf values and includes them in the line list whenever they appear more reliable than the current data. He is currently generating new line lists for all elements for use in computing spectra. These will be either upgrades to his existing line data that we have been using in the work described here or extensions to new elements and higher stages of ionization. As a byproduct of the new work, Kurucz will be able to generate model atoms of arbitrary complexity as we need them for non-LTE calculations.

For each ion Kurucz computes all the allowed and forbidden transitions (that will fit in his workstation). Radiative, Stark, and van der Waals damping constants and Landé g values are automatically produced for each line. The computed eigenvalues are replaced by the laboratory energy levels when known so that lines between known levels have reliable wavelengths.

Kurucz recomputes the energy levels and line lists whenever new spectroscopic analyses become available, and he provides predicted line data to laboratory spectroscopists and observers.

4. Kurucz Web Site and CD-ROMs

Kurucz has set up a web site, KURUCZ.HARVARD.EDU, making available his computer programs, atomic and molecular line lists, the details of the new atomic and molecular calculations, opacities, model atmospheres, predicted spectra, predicted solar irradiance, solar atlases, etc.

Kurucz also publishes his programs and data on CD-ROMs. (Many of the files are too large for easy internet transport.) In the last year he has produced CD-ROM 24 with a TiO linelist and CD-ROMs 25 and 26 with $\rm H_2O$, all using data from Schwenke and Partridge at Ames. These should be useful for interpreting sunspot spectra.

5. Atlases

Kurucz produces detailed solar atlases to test the calculated solar spectra and transmitted spectra. He identifies problems with the line data and he tries to make generic corrections that improve hundreds or thousands of lines at a time. If the spectrum calculations look good in the regions of high transmission through the Earth's atmosphere, there can be some confidence that the regions of low transmission are also

computed reliably. The main problem has been the determination of the reference continuum which affects the appearance of line wings and the apparent depth of weak features.

Kurucz is producing atlases of the solar flux, central intensity, and limb intensity from 0.3 to 5 μ m using FTS spectra taken by James Brault at Kitt Peak. For these, and for several sets of ultraviolet spectra, Kurucz will produce print-on-demand atlases that include a computed spectrum and the line identifications. The observed spectrum will be given relative to a prescribed absolute continuum level, and the current state-of-the-art computed spectrum will be given with and without absorption by terrestrial lines. In many wavelength regions the observed spectrum is not well represented by the calculated spectrum, as noted below. The observed and calculated spectra and line identifications are color coded in each atlas panel. The high resolution printed versions of these atlases will be distributed to research centers. The data will be made available on the web site and on CD-ROMs.

Kurucz is now able to compute a line-blanketed, radiative and convective equilibulum solar photospheric model (see Kurucz 1992a, b, c) that reproduces the irradiance measurements of Neckel and Labs (1984) in the visible for bandpasses of approximately 2 nm. That model, and the empirical quiet-Sun model of Fontenla, Avrett, and Loeser (1993) that includes the chromospheric temperature rise can be used to predict the quiet-Sun irradiance out to 200 μ m. He has computed the spectrum from 150 nm to 200 μ m for both these models at a resolving power of 500,000 using all 58 million lines, i.e., including lines at both known and predicted wavelengths. The computed spectra are not reliable in detail because many lines are at the wrong wavelengths, but when degraded to a resolving power of 10,000 or less the computed spectra agree with Neckel and Labs. In regions of low transmission, the computations give a more reliable solar spectrum than can be obtained from ground-based observations. These low resolution spectral irradiances have been included in the MODTRAN program for use in terrestrial atmospheric modeling. They are available on Kurucz' web site.

For wavelength regions in which the ground-based observed flux is partly obscured by terrestrial lines, Kurucz is calculating and removing the terrestrial line absorption, using the theoretical solar spectrum determined with accurate line data to fill in heavily obscured regions. In this way Kurucz expects to produce an atlas showing for the first time the true solar flux spectrum at high spectral resolution from 0.3 to $5~\mu m$. Such high resolution spectral irradiances are needed in studies of the molecular chemistry of the Earth's upper atmosphere.

6. Summary

We are trying to develop comprehensive modeling techniques that are accurate enough to calculate solar spectra which match accurate observations, and which can fill in wavelength gaps between fragmentary observations. Our purpose is to understand both the solar atmosphere and the solar spectrum. We have been working on this complex task for many years and have made much progress in understanding the basic structure of quiet and active regions.

A major physical problem still to be solved is to understand the time variability of various atmospheric parameters in response to waves traveling through the atmosphere. We believe that including such local variations can resolve the apparent inconsistency between time-averaged observations of the strong infrared CO lines that do not show any chromospheric temperature increase and other diagnostics that clearly indicate an increasing chromospheric temperature with height.

Our research consists of two interrelated efforts: further development and application of the Pandora conputer program for basic physical modeling, and the

continuation of Kurucz's extensive work on line opacities, spectrum simulations, and detailed comparisons with observed solar spectra.

The solar spectrum observed at high spatial and temporal resolution contains a wealth of information that can be used to determine the properties of the emitting regions. We expect to produce models that are more realistic than those now available, that will provide good agreement between calculated and observed spectra.

As a result, we should be able to provide reliable calculated spectra for the brightness components of various quiet and active regions located at different heliocentric angles on the solar disk. Given images of the disk at a particular time showing the location of the different component regions, the high-resolution calculated spectra can be used to construct the corresponding image at any wavelength for that time, and an integration over the disk gives the corresponding spectral irradiance. Lower resolution irradiance is constructed by integrating over a low resolution bandpass. Our recent results on this project have been reported by Fontenla, White, Fox, Avrett, and Kurucz (1999).

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